Complementary Quantum Mechanics

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Lectures: Tuesdays 11:00 – 12:00 in 8.2.04
Thursdays 11:00 - 12:00 in 8.2.02

Practical classes: Thursdays 12:00AM – 13:00PM in 8.2.02
Not obligatory, in a form of tutorials

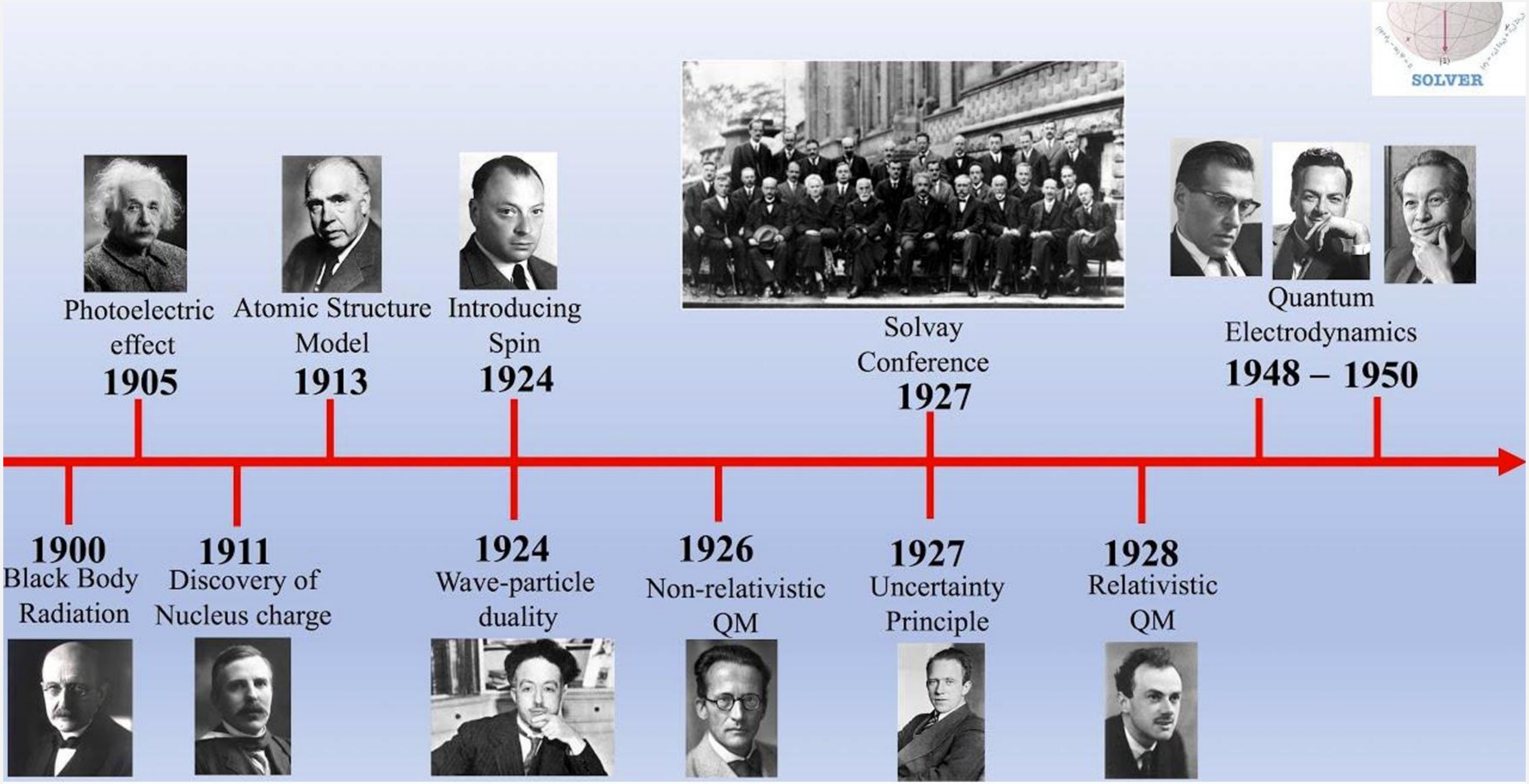
Evaluation: 60% Test1 & Test2+ 40% Project&Presentation

Topics

- Review of Quantum Mechanics concepts and instruments
- Approximation methods
- Basics of quantum computing
- Elements of scattering theory
- Identical Particles
- Groups and Symmetries

1: Review of Quantum Mechanics concepts and instruments

Timeline of the development of Quantum Mechanics



Quantum Mechanics

Classical mechanics does not work on the “small” scale of matter:

- Black Body radiation
- Photoelectric and Compton Effects
- Atomic spectra
- Electron diffraction from crystals

Between 1926 and 1927 by Schrödinger, Heisenberg and Born finally obtained a consistent description of matter on small scale and is as is known as “Quantum Mechanics”

Bohr Correspondence principle: Quantum theory must reduce to classical mechanics on a larger scale and/or large quantum numbers.

Q: What is “small” ?

1. De Broglie’s wavelength $\lambda_b \sim h/p \sim$ obstacles $\Rightarrow$ small
2. Angular momentum ≤ Planck’s constant h

Ang. Mom. of earth $\sim 10^{68}\, h$

Ang. Mom. of molecules $\sim h$

Ang. Mom. of a bicycle wheel $\sim 10^{32}\, h$

Ang. Mom. of nuclei $< h$

1.1: Postulates of Quantum Mechanics: Copenhagen interpretation

The **six postulates** of quantum mechanics (Copenhagen interpretation)

1. The wavefunction
2. Operators in Quantum Mechanics: Connection between observables and mathematical operators
3. The superposition postulate
4. The expansion postulate
5. Measurements in quantum mechanics
6. Time evolution of the wavefunction

1- The Wavefunction

Postulate 1: For every dynamical system, there exists a wavefunction Ψ that is **a continuous, square-integrable and single valued function of all the particles coordinates and time and from which all possible predictions of the physical properties of the system can be obtained.**

Requirements for wavefunction

Wavefunction must satisfy **3 Conditions:**

1. Wavefunction must be a **continuous (No jumps in Ψ (x,t)), finite, single-valued** function of position and time.

To ensure that $|\Psi(x,t|^2$ is uniquely defined as $p \propto |\Psi(x,t|^2$ unique.

2. The integral of the squared modulus of the wavefunction all values of x must be **finite**.

$$\int_{\text{space}} |\Psi(x,t)|^2 dx \;\; = \text{finite number}$$

To allow the wavefunction to be normalised.

1. Derivative $\frac{\partial\Psi(x,t)}{\partial x}$ must be continuous **(no-kinks in Ψ (x,t)** everywhere except where potential is discontinuous (ie for finite potential).

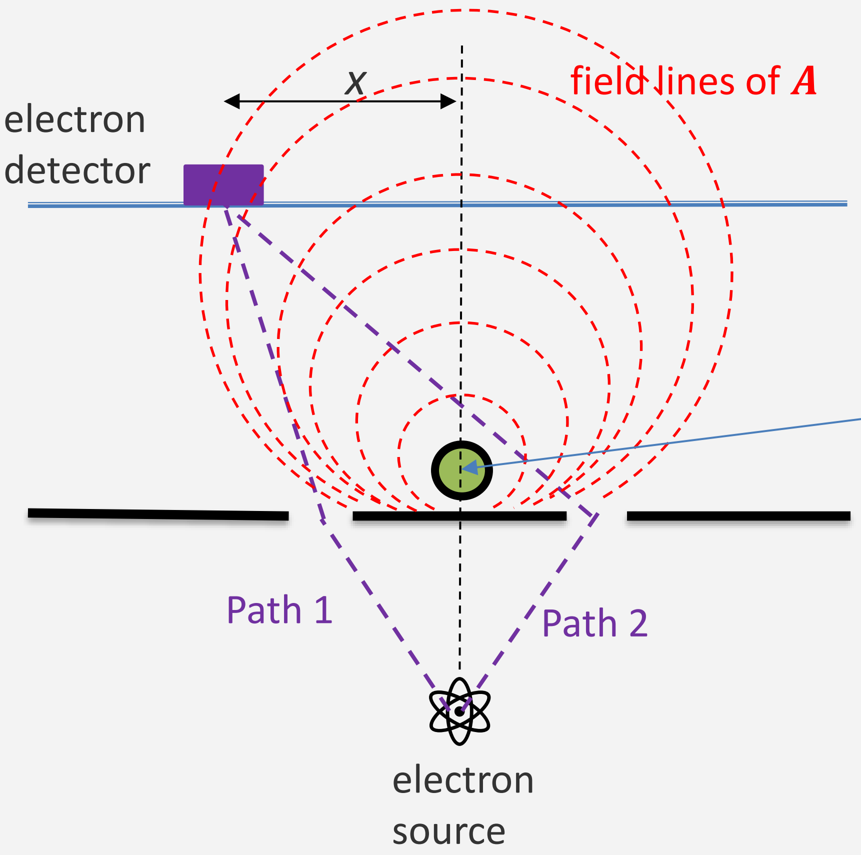
The phase of a wave function: examples

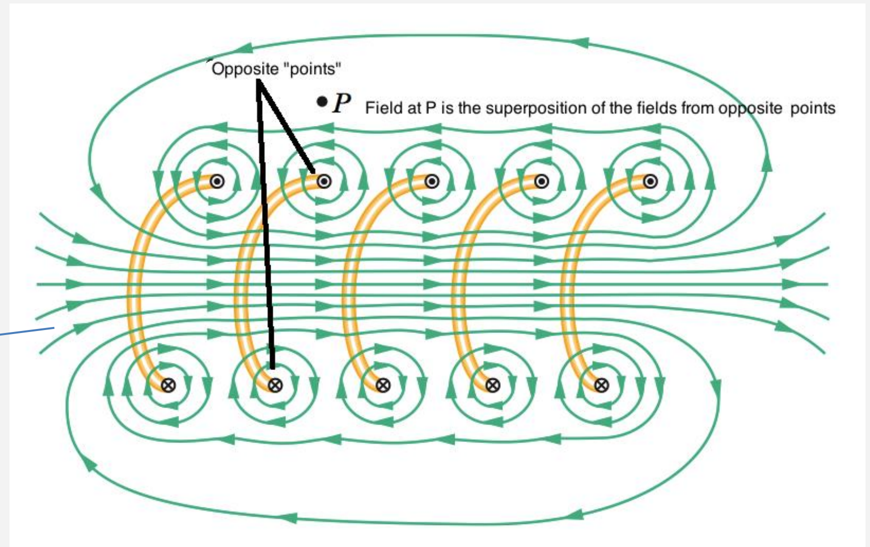
Now we discuss several experiments which demonstrate the role of the phase of the wave function. These emphasize that the fundamental quantity in quantum mechanics is the wave function Ψ and not its absolute value $|\Psi|^2$, i.e

$$\Psi(x,t) = |\Psi(x,t)|e^{i\delta(x,t)}$$

Aharonov–Bohm effect (1949-59)

- A phenomenon in which an electrically charged particle is affected by an electromagnetic potential $(\phi, \boldsymbol{A})$, despite being confined to a region in which both the magnetic field $\boldsymbol{H}$ and electric field $\boldsymbol{E}$ are zero.





https://physics.stackexchange.com/questions/102312/what-are-the-limits-of-validity-for-the-magnetic-field-of-a-solenoid

- Wave function of a free particle $\Psi(\mathbf{r}, t) = \mathrm{C} \exp\left(-\frac{i}{\hbar} Et + \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}\right)$

- In electrodynamics magnetic field can be included by the following replacement in the Hamiltonian (energy density):

$$\mathbf{p} \rightarrow \mathbf{p} - e\boldsymbol{A}/c$$

- This changes the phase of the wave function as:

$$\frac{\mathbf{p} \cdot \mathbf{r}}{\hbar} \rightarrow \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar} - \frac{e}{\hbar c} \int \boldsymbol{A} \cdot d\mathbf{r}$$

- Such that the electron arriving at the detector gains an additional phase difference

$$\Delta\delta = \left(-\frac{e}{\hbar c} \int_1 \boldsymbol{A} \cdot d\mathbf{r}\right) - \left(-\frac{e}{\hbar c} \int_2 \boldsymbol{A} \cdot d\mathbf{r}\right) = \frac{e}{\hbar c} \oint \boldsymbol{A} \cdot d\mathbf{r}$$

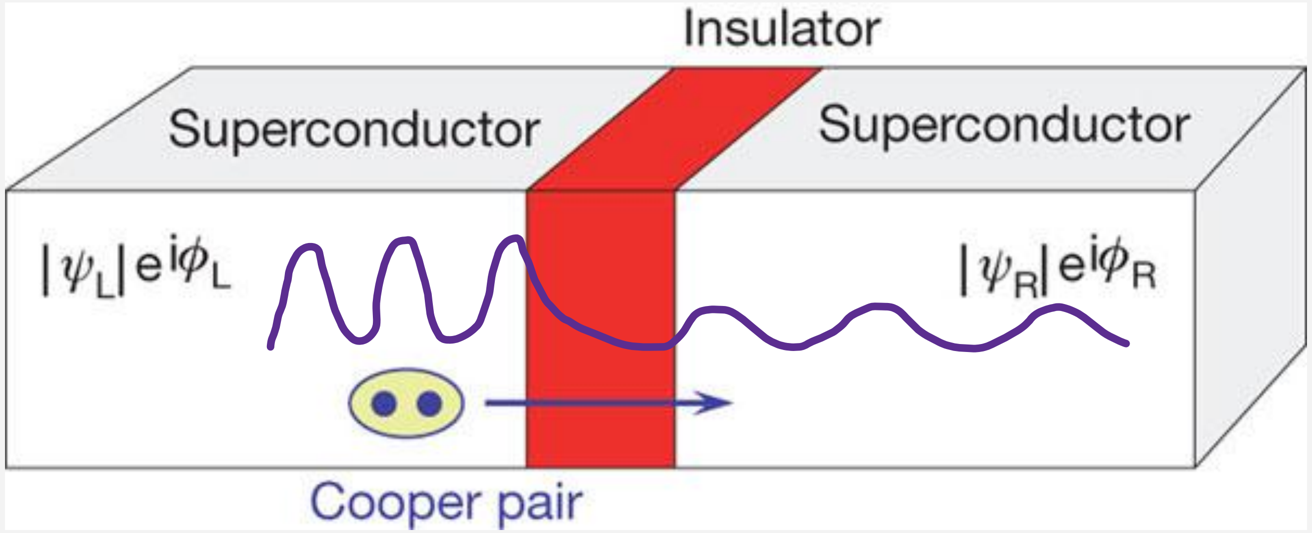
- Using Stokes theorem $\Delta\delta = \iint \boldsymbol{\nabla} \times \boldsymbol{A}\, ds = \frac{e}{\hbar c}\Phi$, where Φ is the magnetic flux trough the surface bounded by the contour composed of Path 1 + Path 2
- Therefore the interference patterns shifts

$$I = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos(\delta + e\Phi/\hbar c)$$

- Conclusions: i) the phase of the phase function can be measured ii) the vector potential $\boldsymbol{A}$ also has direct measurable consequences

Josephson effect (1962-63)

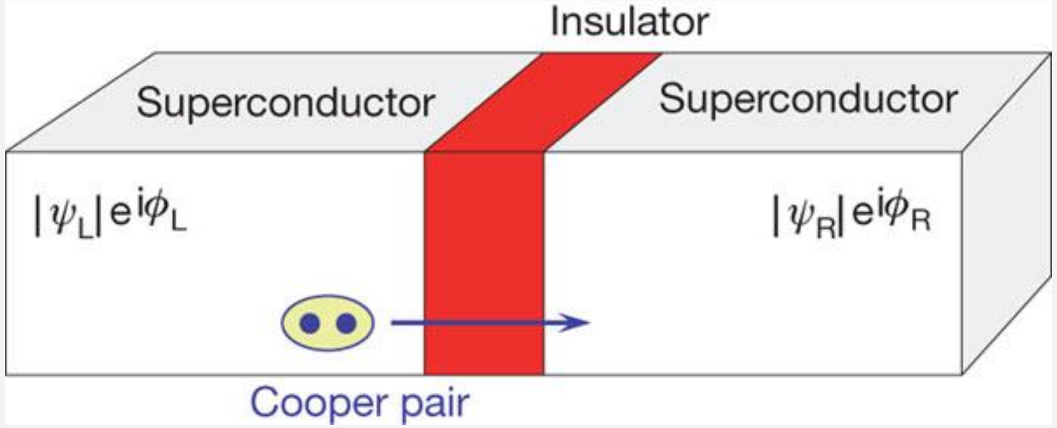
- Two superconductors separated by a thin insulating layer can experience tunnelling of ***Cooper pairs of electrons*** through the junction. In the stational Josephson effect, a current proportional to **sin** of the **phase difference** of the wavefunctions can flow in the junction in the absence of a voltage.



You & Nori (2011), Nature 474, 589−597

Stationary case, no voltage: $J = J_0 \sin(\phi_L - \phi_R)$

Josephson effect (1962-63)



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Non-stationary case, with constant electric potential difference:

In electrodynamics electrostatic potential can be included by replacement $E \to E - e\varphi,$ therefore the wave function phase

$$\frac{E}{\hbar}t \to \frac{E}{\hbar}t - \frac{2e}{\hbar}\int \varphi dt$$

$$J = J_0 \sin(\phi_L - \phi_R - \frac{2eV}{\hbar}t)$$

2-Operators and dynamical variables

Postulate 2a: Every dynamical variable A (such as position, momentum….) is represented by a **linear and Hermitian** operator $\hat{A}$

Properties of Hermitian Operators

- Expectation (average) value is real ie $\langle \hat{A} \rangle = \langle \hat{A} \rangle^*$

- Eigenvalues of Hermitian operators a_n are real. ie $a_n = a_n^*$

Eigenvalue a_n of state n

Recall: Eigenvalue equation

Operator $\hat{A}$

$$\boxed{\hat{A}\psi_n = a_n\psi_n}$$

Eigenfunction ψ_n

Eigenvalues of the Hermitian operators are real and thus physically realisable. In other words that the measured quantities are real .

- Eigenfunctions are orthonormal ie $\int_{space} \psi_m^* \psi_n dV = \delta_{n,m}$ **eq. 1**
- If ψ_n satisfy **eq. 1**, they are said to form a **complete set**

Linear operators

All operators used in quantum mechanics **are linear**

Definition: An operator $\hat{\mathrm{A}}$ **is linear only and only if**:

$$\widehat{\mathrm{A}}(\mathrm{a}\psi_1 + b\psi_2) = a\widehat{\mathrm{A}}\psi_1 + b\widehat{\mathrm{A}}\psi_2$$

(where ψ_1 and ψ_2 are two wavefunctions and a and b are any two constant)s

Eg: $\hat{A} = \frac{d}{dx}$ is linear but $\hat{B} = \ln x$ is not linear

Hermitian operators

Take two wavefunctions ψ_m and ψ_n that a given operator $\hat{A}$ can act on.

Definition: An operator is **Hermitian** only and only if:

For all values of m and n :

$$\int \psi_m^* \hat{A} \psi_n dV = \int (\hat{A}\psi_m)^* \psi_n dV = \left(\int \psi_n^* \hat{A} \psi_m dV \right)^* \quad \textbf{Hermiticity condition}$$

$$\boldsymbol{A_{mn}} \quad = \quad (\boldsymbol{A_{nm}})^*$$

eq.7

- Define the **matrix element**: $A_{mn} = \int \psi_m^* \hat{A} \psi_n dV$
- In matrix notation eq 7: Hermiticity condition becomes $\boldsymbol{A_{mn}} = (\boldsymbol{A_{nm}})^*$

RHS: Complex Conjugate transpose matrix elem

Properties of Hermitian operators

If an operators is Hermitian then it satisfy the following:

1. Its eigenvalues are **always real**
2. Its corresponding **eigenfunctions are orthogonal**
3. It expectation values **are always real**

Very important in QM as it ensures that the eigenvalues are physically realisable

Example

Show that the momentum operator $\hat{p}_x = -i\hbar\frac{d}{dx}$ is Hermitian

Operators and expectation values

Definition: Expectation (average) value of A as $\langle A \rangle$ obtained after a large number of measurements on identical particles

$$\text{Expectation value: } \langle A \rangle = \frac{\int_{space} \Psi^*(x,t)\hat{A}\Psi(x,t)dx}{\int_{space} \Psi^*(x,t)\Psi(x,t)dx}$$

eq.5

$\hat{A}$ is operator associated with A.

- If $\psi(x)$ is normalised:

$$\int_{space} \Psi^*(x,t)\Psi(x,t) = \int_{space} |\psi(x)|^2 dx = \int_{space} p(x)dx = 1.$$

$$\Rightarrow \quad < A >= \int_{space} \Psi^*(x,t)\hat{A}\Psi(x,t)dx$$

$\Psi^*(x,t)\hat{A}\Psi(x,t)$: First evaluate $\hat{A}\Psi(x,t)$, then multiply the result with $\Psi^*(x,t)$

3- The superposition postulate

Postulate 3: Any linear **combinations (superposition)** of two or more **eigenfunctions** of a given operator Â may be used to build up a new **wavefunction** Ψ **which is also a possible state** of the system such:

$$\boldsymbol{\Psi(r) = c_1\psi_1 + c_2\psi_2 + \cdots + c_s\psi_s = \sum_{n}^{s} c_n\psi_n}$$

Quantum superposition;

Later in quantum computing

(eq. 2)

- $\psi_1, \psi_2, \ldots \psi_s$: *are allowed wavefunctions (states) of the system*
- *Each state n satisfies* $\hat{A}\psi_n = a_n\psi_n$
- s may go to ∞ and $c_1, c_2 \ldots c_n$: coefficients (real or complex)
- $c_1, c_2 \ldots c_n$: Define composition of the state $\Psi(r)$. Unique for that state
- **When in a superposition state and not measured** particle is a wave and **exists in multiple states at once (at the same time)**: Recall: particle goes through both slits at the same time in double slit experiment when not measured
- Different from classical superposition

4: The expansion principle

Postulate 4: Any arbitrary wavefunction Ψ can be expanded as a **unique linear superposition of a complete, orthogonal set** of eigenfunctions of any Hermitian operator as:

$$\boxed{\Psi = \sum_{n}^{s} c_n \psi_n} \quad \text{with} \quad \boxed{c_n = \int_{-\infty}^{+\infty} \psi_n^* \Psi \, dx} \qquad \text{(eq. 4)}$$

Notes:

- Ψ has the **same** boundary conditions as ψ_n
- Expansions is generalisation of Fourier Series.
- Very useful, as can, in principle, any arbitrary wavefunction using eigenfunctions of whichever observable we want to measure.

5-The measurement postulate

Postulate 5a: In any measurement of the dynamical variable (observable) associated with an operator Â, the **only values that will ever be measured are the eigenvalues a_n *associated with that observable.***

Captures the central point of quantum mechanics

Two possible cases:

Case 1: If the system is in an eigenstate ie $\hat{A}\psi_n = a_n\psi_n$

$\Rightarrow$ Results of measurement will be eigenvalue a_n.

$\Rightarrow$ Probability associated with measurement $p_n = 1$

Example: Take SHO in its ground state $\psi_0 = (\alpha/\pi)^{1/4}e^{-\frac{\alpha x^2}{2}}$ $\alpha = \frac{m\omega}{\hbar}$

Satisfies eigenfunction equation $\hat{H}\psi_0 = E_0\psi_0 = \frac{1}{2}\hbar\omega\psi_0$

Energy Measurements: If the system is in state ψ_0, the **only possible result** of measuring the particle's energy is the corresponding eigenvalue energy $E_0 = \frac{1}{2}\hbar\omega$.

Measurements (ctd)

Case 2: If the system is in **superposition state** described by a wavefunction $\Psi = \sum_n^s c_n \psi_n$

Ψ is not an eigenstate of $\hat{A}$.

Question: What are results of measurements of measuring observable associated with $\hat{A}$?

Postulate 5 $\Rightarrow$ *only eigenvalues of* $\hat{A}$ *can be obtained* $\Rightarrow$ *One eigenvalue in a measurement so one state*

- When in a superposition state: **Before measurement**, system exists in **multiple states at once**.
- **When measured**: Find only **a single state**

Measurement: Expectation value

- ***Postulate 5⇒ only eigenvalues of*** $\hat{A}$ ***can be obtained*** in any measurement
- Possible outcomes will be $a_1, a_2 \ldots a_s$
- **Associate a probability** with each measurement yielding an eigenvalue a_n:

$$\boxed{p_n = \text{probability of obtaining } a_n} \quad (5)$$

- Satisfies: $\sum_{n=1}^{s} p_n = 1$
- Expectation (average value): $$\boxed{\langle A \rangle = \sum_{n}^{s} p_n a_n,} \quad (6)$$

(weighted average of a_n)

On the other hand $\langle A \rangle = \int \Psi^* \hat{A} \Psi dV = |c_1|^2 a_1 + |c_2|^2 a_2 + \cdots + |c_s|^2 a_s \ \rightarrow p_n \equiv c_n^* c_n$

Measurement (4): Collapse of wavefunction

Postulate 5b: Immediately after the measurement, the wavefunction of the particle is an eigenfunction of the operator corresponding to the eigenvalue just obtained as the measurement result.

$$\boxed{\Psi = \sum_{n=1}^{s} c_n \psi_n \longrightarrow \Psi = \psi_n}$$

- This is known as the **collapse of the wavefunction**
- **This is the Copenhagen Interpretation**

- Assume that the result of the first measurement yields an eigenvalue a_i and corresponding wavefunction ψ_i with a probability $p_i = |c_i|^2$
- If we re-measure the same quantity **immediately after first measurement** and would obtain again a_i (wavefunction collapses to ψ_i) with a probability $\mathrm{p}_i = 1$

Measurement example

Consider a particle in a Simple Harmonic potential with following wavefunction:

$$\Psi(x,0) = \frac{1}{3}\left(\sqrt{3}\psi_0(x) + 2\psi_1(x) + \sqrt{2}\psi_2(x)\right)$$

Where ψ_0, ψ_1 are 3 lowest orthonormal states corresponding of the SHO with corresponding energies $E_n = (n + ½)\hbar\omega$ corresponding to $n = 0, 1$ and 2 respectively and $c_n = 0\ for\ n \geq 3$.

Homework question:

1. Calculate the probability of finding the particle in anyone of the states ψ_0, ψ_1 and ψ_2. Verify that the total probability is equal to 1.
2. What are possible values of energy of the particles?
3. Consider an ensemble of 810 identical particles, each of them is in the state ⍰(x). If the measurements are done on all of them, how many will be found in each of these states?
4. What would be the average value of the energy?

Uncertainty

- QM can also predict **standard deviation ΔA** of a set of measurements as a measure of the spread around average value <A>.
- Predicted standard deviation is **uncertainty** in the value of the variable.
- Defined as: $\Delta A = \sqrt{< A^2 > - < A >^2}$

Where $\langle A \rangle$ is given by eq 4 and and $< A^2 >= \dfrac{\int_{space} \Psi^*(x,t)\hat{A}^2\Psi(x,t)dx}{\int_{space} \Psi^*(x,t)\Psi(x,t)dx}$

- Most commonly used are uncertainty in energy ΔE , momentum Δp, position Δx and time Δt to give Heisenberg's relations

The Schwarz inequality

Take two operators $\hat{A}$ and $\hat{B}$

- Let ΔA and ΔB the uncertainty associated with measuring A and B

$A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$ and $\Delta B = \sqrt{\langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2}$ (Standard deviations)

Where $\langle \hat{A}^2 \rangle = \int \psi^* \hat{A}^2 \psi \, dV$; $\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, dV$.

- Then ΔA and ΔB satisfy the Schwarz inequality

$$\boxed{\Delta A . \Delta B \geq \frac{1}{2} \left| \left\langle [\hat{A}, \hat{B}] \right\rangle \right|} \quad \text{eq.8}$$

Where $\langle [\hat{A}, \hat{B}] \rangle = \int \psi^* [\hat{A}, \hat{B}] \psi \, dV = \int \psi^* (\hat{A}.\hat{B} - \hat{B}.\hat{A}) \psi \, dV$

Consequence: Uncertainty principle

$$\boxed{\Delta A . \Delta B \geq \frac{1}{2}\left|\langle[\hat{A}, \hat{B}]\rangle\right|}$$

If $\hat{A}$ and $\hat{B}$ <u>commute</u> ie $[\hat{A}, \hat{B}] = 0$ $\quad \Delta A.\Delta B \geq 0$ $\quad \Rightarrow$ No inconsistency in having both ΔA and ΔB zero, ie can have

ie can have $\Delta A = 0$ <u>and</u> $\Delta B = 0$ at the same time

If $\hat{A}$ and $\hat{B}$ <u>do not commute</u> ie $[\hat{A}, \hat{B}] \neq 0$

So, if $\Delta A = 0 \Rightarrow \Delta B$ has to infinite (ΔA and ΔB related)

Properties of commuting operators

- Consider two operators $\hat{A}$ and $\hat{B}$ that commute i.e:

$[\hat{A}, \hat{B}] = 0 \Rightarrow \hat{A}.\hat{B} = \hat{B}.\hat{A} \Rightarrow \hat{A}.\hat{B}(\phi) = \hat{B}.\hat{A}(\phi)$ (ϕ: any given wavefunction)

Conclusions: If two operators commute:

1. They **must** share the **same eigenfunctions** but have **different eigenvalues**
2. Simultaneous and precise measurements can be made on their corresponding **observables** .

Consequences: Simultaneousity and Complementarity

Take two given observables.

Suppose we require to do simultaneous measurement on both. What results of measurements?

Two cases:

1. If two observables are to have simultaneously precise values (ie can measure both with infinite precision at the same time) $\Rightarrow$ their corresponding operators **must commute ie** $[\hat{A}, \hat{B}] = 0$

   Ie: simultaneous measurements (infinite precision for both)
2. If corresponding operators **do not commute ie** $[\hat{A}, \hat{B}] \neq 0$

   $\Rightarrow$ Cannot make infinitely and simultaneously precise measurements on both

Example of commuting operators

Eg: Take Hydrogen atom

Electron's angular momentum described by: $\hat{L} = [\hat{L}_x, \hat{L}_y, \hat{L}_z]$ 3 components

with $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.

Eigenvalues of $\hat{L}$ *and* $\hat{L}_z$ are common (the same)

and they are known as **Spherical Harmonics .**

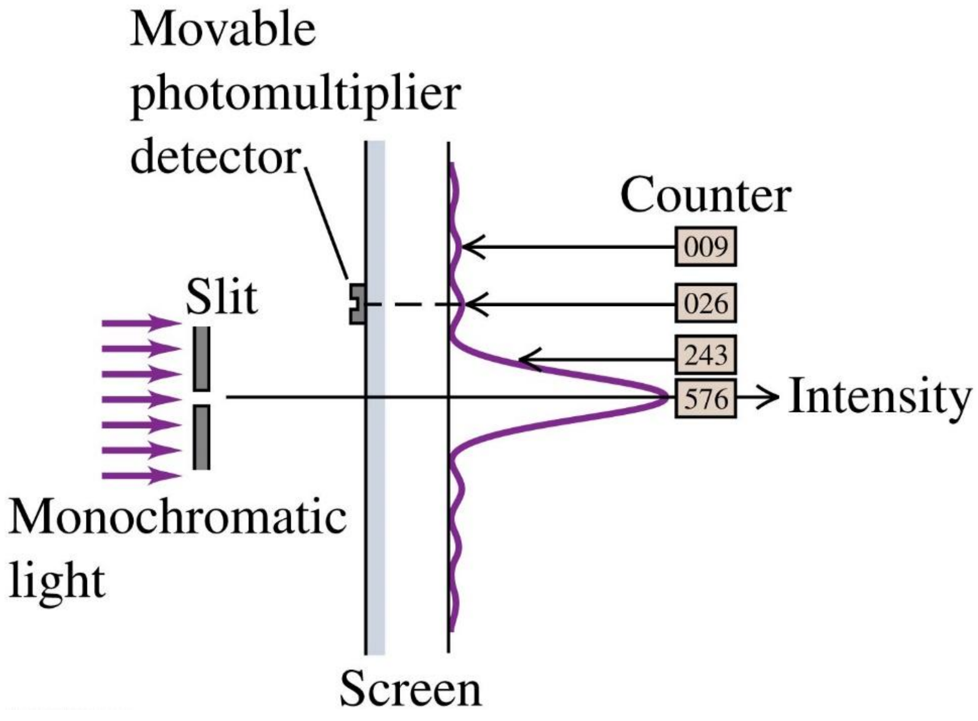
$$i.e: \ \hat{L}^2 Y_{\ell,m_\ell}(\theta,\varphi) = \hbar^2 \ell(\ell+1) Y_{\ell,m_\ell}(\theta,\varphi) \qquad 0 \le \ell \le n-1$$

$$\hat{L}_z Y_{\ell,m_\ell}(\theta,\varphi) = m_\ell \hbar Y_{\ell,m_\ell}(\theta,\varphi) \qquad -\ell \le m_\ell \le +\ell$$

Possible because $\hat{L}$ *and* $\hat{L}_z$ commute is: $[\hat{L}^2, \hat{L}_z] = 0$

Photon Diffraction and Uncertainty (1 of 2)

- When a photon passes through a narrow slit, its momentum becomes uncertain, and the photon can deflect to either side.
- A diffraction pattern is the result of many photons hitting the screen.
- We can’t predict the exact trajectory of an individual photon, we can only describe the probability that an individual photon will strike a given spot on the screen.



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- This fundamental indeterminacy has no counterpart in Newtonian mechanics.

Probability and Uncertainty (2 of 2)

- Assume that $\lambda \ll a$. Fraunhofer's diffractions $\Rightarrow$ $\sin\theta_1 \approx \theta_1 = \lambda/a$.

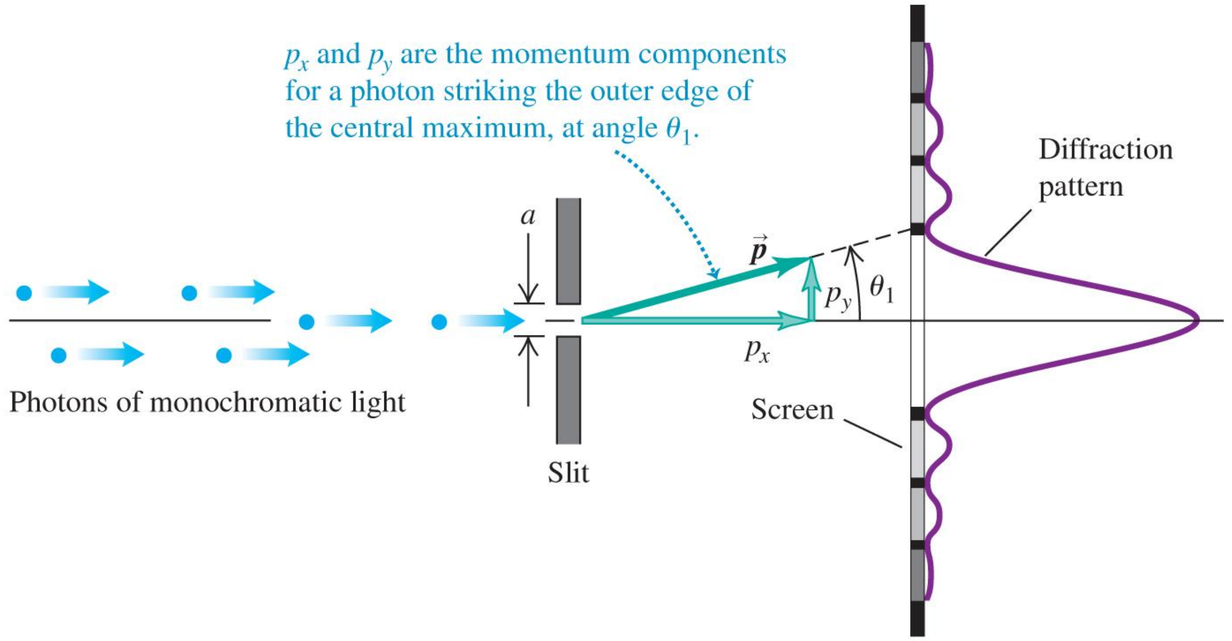
- $p_y = p_x \tan\theta_1 \approx p_x\theta_1 = \frac{p_x\lambda}{a}$.

- The photons that contribute to the central maximum, have y-component of the momentum, spread over a range from $-\frac{p_x\lambda}{a}$ to $\frac{p_x\lambda}{a} \Rightarrow$

- There will be an uncertainty Δp_y in the y-component of the momentum:

$$\Delta p_y \geq \frac{p_x\lambda}{a} \approx \frac{p_x h}{p_x a} = \frac{h}{a} \Rightarrow$$

$$\Delta p_y a \geq h\,.$$



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- The slit width a represents an uncertainty in the y-component of the position of a photon as it passes through the slit.

6-Time evolution of a system

Postulate 6: Between measurements (when the system is not disturbed by any external influence), the time evolution of the system is described by **time dependent Schrödinger equation**:

$$\hat{H}\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t}$$

Assume 3D

Consider case where **Hamiltonian $\hat{H}$ is independent of time.**

Two cases

Case 1: If ψ_n is an eigenstate of $\hat{H}$: $\hat{H}\psi_n = E_n\psi_n$

- The time dependent wavefunction:

$$\boxed{\Psi(r,t) = \psi_n(r)\exp\left(\frac{-iE_nt}{\hbar}\right)}$$

where the term $e^{-iE_nt/\hbar}$ gives the time dependence

6-Time evolution of a system (ctd)

Case 2: If wavefunction is a superposition of states (**not** an eigenstate of $\hat{H}$) and can be expanded as:

$$\Psi(r) = \sum_{n}^{s} c_n \psi_n(r)$$

- Take $c_n \rightarrow c_n(t=0)e^{-iE_n t/\hbar} \Rightarrow$

- The time evolution (dependence) given by:

$$\boxed{\Psi(r,t) = \sum_{n}^{s} \psi_n(r) \underbrace{c_n(0)e^{-iE_n t/\hbar}}_{c_n(t)}}$$

$$\Rightarrow \Psi^*(r,t) = \sum_{n}^{s} \psi_n^*(r) c_n^* e^{iE_n t/\hbar}$$

Time dependence of superposition state example

Take another example of an SHO potential with wavefunction:

$$\Psi(x) = \frac{1}{\sqrt{7}}\left(2\psi_0(x) + \sqrt{3}\psi_1(x)\right)$$

- At any later time t we obtain:

$$\Psi(x,t) = \frac{1}{\sqrt{7}}\left(2\psi_0(x)e^{-iE_0t/\hbar} + \sqrt{3}\psi_1(x)e^{-iE_1t/\hbar}\right)$$

- Complex conjugate $\Psi^*(x,t)$

$$\Psi^*(x,t) = \frac{1}{\sqrt{7}}\left(2\psi_0^*(x)e^{iE_0t/\hbar} + \sqrt{3}\psi_1^*(x)e^{iE_1t/\hbar}\right)$$

- **Exercise**: Show that

$$|\Psi(x)|^2 = \Psi^*(x,t) \times \Psi^*(x,t) = \frac{1}{7}\left(4\psi_0^2(x) + 3\psi_1^2(x) + 4\sqrt{3}\psi_0(x)\psi_1(x)\cos\left((E_1 - E_0)t/\hbar\right)\right)$$

Summary

- Wavefunction to represent state of system.
- Hermitian operators to represent dynamic variables: $\hat{A}\psi_n = a_n\psi_n$
- Eigenvalues a_n are **real:** $a_n = a_n^*$
- Eigenfunctions ψ_n are orthonormal: $$\boxed{\begin{aligned}\int \psi_m^*\psi_n dV &= 1 \quad \text{if } n = m \\ &= 0 \quad \text{if } n \neq m\end{aligned}}$$
- Superposition of wavefunctions. $\Psi(r) = \sum_n^s c_n\psi_n(r)$
- Normalisation: $\sum_{n=1}^s |c_n|^2 = 1$
- **Only** allowed outcomes of measurements are **eigenvalues** of operator.
- **Several** possible outcomes with associated probabilities.: $p_n = |c_n|^2$
- Probability p_n of measurement yielding eigenvalue a_n
- Average value of observable: $\langle A\rangle = \sum_n^s |c_n|^2\, a_n = \sum_n^s p_n a_n$
- Time dependence solution

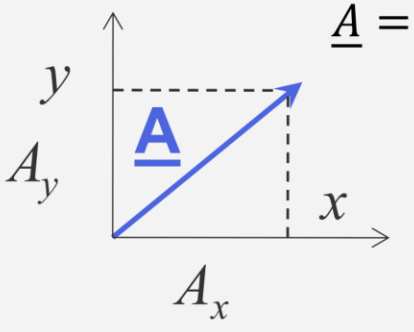
$$\boxed{\hat{H}\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t}} \qquad \boxed{\Psi(r,t) = \psi(r)\exp-\frac{iE_nt}{\hbar}} \qquad \boxed{\Psi(r,t) = \sum_n^s \psi_n(r)c_n\exp-\frac{iE_nt}{\hbar}}$$

1.2: The Dirac notation

Quantum states as vectors

Vector Algebra: 2D or 3D space with orthonormal unit vectors.

- Linear combination of vectors:



$\underline{A} = A_x\underline{i} + A_y\underline{j}$

$$\boldsymbol{A} = \sum_i A_i \boldsymbol{u}_i$$

- Scaler (dot) product: $\boldsymbol{u_i}.\boldsymbol{u_j}$
- Unit vectors form **a basis**: are orthonormal ie satisfy: $\boldsymbol{u_i}.\boldsymbol{u_j} = \boldsymbol{\delta_{ij}}$
- j^{th}component of the vector:

$$= \boldsymbol{u_j}.\sum_i A_i \boldsymbol{u_i} = \sum_i A_i \underbrace{\boldsymbol{u_j}.\boldsymbol{u_i}}_{=\delta_{ij}} = A_j$$

$$\therefore A_i = \boldsymbol{u_i}.\boldsymbol{A}$$

Quantum Analogue

- Linear combination of wavefunctions:

$\Psi(x) = \sum_n^s c_n\psi_n(x)$: c_n: coefficient

- Overlap integral (or inner product): $\int_{space}\psi_m^*\psi_n\delta x$
- Wavefunctions are o**rthonormal:**

$$\int_{space}\psi_m^*\psi_n\delta x = \delta_{n,m}$$

- Expansion coefficient c_j: $c_j = \int_{space}\psi_j^*\Psi dx$

Analogy with vectors

Dirac notation: basic ideas

Wavefunctions (or states) of a system described by a complex **state vectors** in the **Hilbert** space that is free of the choice of the coordinate systems but enable us to easily insert a coordinate system.

- State vector represented **symbolically** as ($|\psi\rangle$ **(or** $|\quad\rangle$)): called **"ket"** .
- Complex Conjugate of wavefunction, ψ^* is denoted by the **"bra"** $\langle\psi|$ $or\langle\psi|$.
- **Ket vector** : denotes a state in the abstract form without any reference to any particular representation.

ψ represented by $|\psi\rangle$ **(or** $|\quad\rangle$	**"ket" vector**
ψ^* represented by $\langle\psi|$ or $\langle\psi|$	**"Bra" vector**

Properties of kets, bras and brackets

1. To every (vector) **ket** $|\psi\rangle$ corresponds a **bra** $\langle\psi|$, given by

$|\psi\rangle^\dagger = \langle\psi|$ bra: conjugate of a ket

$\therefore$ There is a **one-to-one correspondence between a bra and a ket.**

$(a|\psi\rangle)^\dagger = a^*\langle\psi|$ (a : complex number)

2. Overlap integral (**scalar or inner product)**

$\int_{\text{space}} \psi^*(x)\phi(x)dx \to \langle\boldsymbol{\psi}|\boldsymbol{\phi}\rangle$ known as **Bracket**

Satisfies: $\langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle$

$\langle\psi|\phi\rangle$: equivalent to multiply ψ^* with ϕ, then integrate over space.

3. $p = |\langle\phi|\psi\rangle|^2$:

$|\langle\phi|\psi\rangle^2|$: interpreted as **probability that** we start with ket $|\psi\rangle$ and end up with bra $\langle\phi|$.

$|\quad\rangle$: Ket $\langle\quad|$: Bra $\langle\quad|\quad\rangle$: Bracket

- **Matrix element A_{mn}** defined as:

$$A_{mn} = \int_{space} \psi_m^* \hat{A} \psi_n dV \xrightarrow{\text{Dirac}} \left\langle \psi_m \middle| \hat{A} \middle| \psi_n \right\rangle = \left\langle m \middle| \hat{A} \middle| n \right\rangle$$

- In this notation, the condition for the operator to be Hermitian is

$$A_{mn} = A_{nm}^* \text{ becomes } \left\langle \psi_m \middle| \hat{A} \middle| \psi_n \right\rangle = \left\langle \psi_n \middle| \hat{A} \middle| \psi_m \right\rangle^* \text{ or } \left\langle m \middle| \hat{A} \middle| n \right\rangle = \left\langle n \middle| \hat{A} \middle| m \right\rangle^*$$

- **Expectation (average value): $\langle \boldsymbol{A} \rangle$**

$$\langle A \rangle = \frac{\int \psi^* \hat{A} \psi dx}{\int \psi^* \psi dx} \xrightarrow{\text{Dirac}} \langle \boldsymbol{A} \rangle = \frac{\langle \boldsymbol{\psi} | \widehat{\boldsymbol{A}} | \boldsymbol{\psi} \rangle}{\langle \boldsymbol{\psi} | \boldsymbol{\Psi} \rangle}$$

Projection operators

Eg: The quantity $\hat{B} = |\phi\rangle\langle\psi|$ is a **linear operator** as **it can act on one ket to give another:**

$$\hat{B}|\psi\rangle = |\phi\rangle\underbrace{\langle\psi|\psi\rangle}_{=1} = |\phi\rangle$$

- Satisfies $\left(|\phi\rangle\langle\psi|\right)^{\dagger} = |\psi\rangle\langle\phi|$
- **Products of type:** $|\psi\rangle\hat{A}$ or $\hat{A}\langle\psi|$ (ie when operator stands to the right of a ket or left of a bra) are forbidden and have no physical meaning

- **Projection operator defined as** $\hat{P}_n = |n\rangle\langle n|$ **:** $\hat{P}$: Hermitian operators that satisfies $\hat{P}^2 = \hat{P}$::

  Eg: projector operator $\hat{P}_n = |n\rangle\langle n|$

$$\hat{P}_n|\Psi\rangle = |n\rangle\langle n||\Psi\rangle = \underbrace{\langle n|\Psi\rangle}_{c_n}|n\rangle = c_n|n\rangle$$

gives component of the state $\psi\rangle$ along direction $|n\rangle$

Completeness rule

If $|n\rangle$ is a discrete orthonormal basis (ie satisfy $(m|n) = \delta_{mn}$), then they satisfy:

$$\boxed{\textstyle\sum_n |n\rangle\langle n| = 1 \quad : \text{completeness rule}}$$

(Operator on RHS: 1=$\hat{I}$ Identity operator))

- **Proof:** $|\Psi\rangle = \sum_n c_n|\psi_n\rangle = \sum_n c_n|n\rangle$: but $c_n = \langle n|\Psi\rangle|$

$|\Psi\rangle = \sum_n c_{n:}\,|n\rangle = \sum_n\langle n|\Psi\rangle|n\rangle = \sum_n|n\rangle\,\langle n|\Psi\rangle$ by inspection:

$$\Rightarrow |\Psi\rangle = \underbrace{\sum_n |n\rangle\,\langle n|}_{\text{must be } 1}\,|\Psi\rangle \Rightarrow \sum_n |n\rangle\langle n| = 1 \quad \therefore \sum_n \hat{P}_n = 1$$

- Since projector operator $\hat{P}_n = |n\rangle\langle n|$:
- Completeness rule: $\sum_n \hat{P}_n = \sum_n|n\rangle\langle n| = 1$
- The sum of all projection operators onto all states of an orthonormal complete set gives identity operator.

Completeness condition: very useful , as it can be incorporated in various places to make calculations easier.

Completeness rule for continuous bases

For a continuous set of basis: expansion expressed in the base of ψ_n becomes:

$$\sum_n c_n \psi_n \xrightarrow{\text{continuous}} \int c(n)\psi(n)dn$$

$$\text{Dirac notation } \Rightarrow |\Psi\rangle = \int c(n)\,\underbrace{|\psi(n)\rangle}_{|n\rangle}\,dn = \int c(n)|n\rangle\,dn$$

- **Completeness rule:** (sum over n becomes integral)

$$\sum_n |n\rangle\langle n| = 1 \xrightarrow{\text{continuum}} \int |n\rangle\langle n| dn = 1$$

- **Orthonormal condition:**

$$\langle m|n\rangle = \delta_{nm} \xrightarrow{\text{continuum}} \langle m|n\rangle = \delta(m-n)$$

Kronecker symbol δ_{nm} is replaced by the **Dirac delta δ-function** (see later)

Position operator in Dirac notation

Position operator: $\hat{x}$

Basis kets of position space written as: $|x\rangle$

Since x $(-\infty \le x \le +\infty)$ continuous variable:

Completeness rule: $\int dx|x\rangle\langle x| = 1$ and $\langle x|x'\rangle = \delta(x - x')$

Dirac notation: $|\Psi\rangle = \underbrace{\int |x\rangle\langle x| dx}_{=1} |\Psi\rangle = \int \langle x|\Psi\rangle |x\rangle dx = \int \Psi(x)|x\rangle dx$

Hence in position representation space wavefunction: $\psi(x) = \langle x|\psi\rangle$
$\psi(x)$ is the component (projection) of the ket $|\psi\rangle$ in position space

Inner product (overlap integral): $\langle\Psi|\Phi\rangle$

$\langle\Psi|\Phi\rangle = \langle\Psi \times 1|\Phi\rangle = \langle\Psi| \int |x\rangle\langle x| dx|\Phi\rangle = \int \overbrace{\langle\Psi|x\rangle}^{=\Psi^*(x)} \overbrace{\langle x|\Phi\rangle}^{\Phi(x)} d\,x = \int \Psi^*(x)\Phi(x)\,dx$ as required

Momentum representation (ie in momentum space)

- Basis $|\hat{p}_x\rangle$ of momentum representation obtained from eigenstates of momentum operator
- Eigenvalue equation: $\hat{p}_x|p_x\rangle = p_x|p_x\rangle$ (p_x: momentum eigenvalue, $|\hat{p}_x\rangle$: momentum eigenvector)

Algebra in this representation can easily inferred from position representation.

- Completeness rule: $\int dp|p_x\rangle\langle p_x| = 1$ and $\langle p_x|p_x'\rangle = \delta(p_x - p_x')$
- Any ket $|\Psi\rangle$ can be expressed in this base as:

$$|\psi\rangle = \underbrace{\int |p_x\rangle\langle p_x|dp_x}_{=1}|\psi\rangle = \int \langle p_x|\psi\rangle|p_x\rangle dp_x = \int \psi(p_x)|p_x\rangle dp_x$$

In momentum representation: space wavefunction $\psi(p_x) := \langle p_x|\psi\rangle$
$\psi(p_x)$ is the component (projection) of the ket $|\psi\rangle$ in momentum space.

- Probability of finding the system momentum in interval Δp_x about given p_x= $|\Psi(p_x)|^2 = |\langle p_x|\psi\rangle|^2$
- Scalar (inner) product in momentum space:

$$\langle\Psi|\Phi\rangle = \langle\Psi|\int|p_x\rangle\langle p_x|dp_x|\Phi\rangle = \int \underbrace{\langle\Psi|p_x\rangle}_{\Psi^*(p_x)}\underbrace{\langle p_x|\Phi\rangle}_{\Phi(p_x)}dp_x = \int \Psi^*(p_x)\Phi(p_x)dp_x\text{: as required}$$

Connecting position and momentum representation

- How do we connect between a state vector in momentum space and a state vector in position space?

Consider $\boldsymbol{\psi(x) = \langle x|\psi\rangle}$

$$\psi(x) = \langle x|\psi\rangle = \langle x|1|\psi\rangle = \langle x|\int |p_x\rangle\langle p_x|dp_x|\psi\rangle = \int \langle x|p_x\rangle \underbrace{\langle p_x|\psi\rangle}_{\Psi(p_x)} dp_x$$

$$\Rightarrow \psi(x) = \int \langle x|p_x\rangle\, \psi(p_x) dp_x$$

$\boldsymbol{\psi(x)}$ and $\boldsymbol{\psi(p_x)}$ are Fourier transforms of each other

- Equally, find that: $\langle x|p_x\rangle = \langle p_x|x\rangle^* = \frac{1}{(2\pi\hbar)^{1/2}} e^{ip_x x/\hbar}$

$$\psi(p_x) = \frac{1}{(2\pi\hbar)^{1/2}} \int \psi(x) e^{-ip_x x/\hbar}\, dx \quad \text{and} \quad \psi^*(x) = \frac{1}{(2\pi\hbar)^{1/2}} \int \psi(p_x) e^{+ip_x x/\hbar}\, dp_x$$

Homework question q1

The Hamiltonian of a certain system is given by:

$$\hat{H} = \alpha\left(|1\rangle\langle 2| + |2\rangle\langle 1|\right)$$

Where $|1\rangle$ and $|2\rangle$ form a complete orthonormal set.

1. Show that $|1\rangle$ and $|2\rangle$ are not eigenstates Ĥ. (hint: evaluate $\hat{H}|1\rangle$ and $\hat{H}|2\rangle$)
2. By considering that eigenstates are given by: $|\Psi\rangle = a_1|1\rangle + a_2|2\rangle$ (a_1 and a_2 constant), Find the normalised eigenstates of Ĥ and their corresponding eigenvalues.

Summary

Wave mechanics

- **Wavefunction:** $\psi(x)$
- Complex conjugate: $\psi^*(x)$
- Modulus squared: $|\psi(x)|^2 = \psi^*(x) \times \psi(x)$
- Complete sets: $\int_{\text{space}} \psi_{\text{n}}^* \psi_m dx = \delta_{nm}$
- Eigenvalue equation: $\hat{A}\psi_n(x) = a_n \psi_n(x)$
- Superposition of states:

$$\Psi = \sum_n c_n \psi_n \rightarrow \Psi^* = \sum_n c_n^* \psi_n^*$$

- Overlap integral: $\int_{\text{space}} \Psi^*(x)\Phi(x)dx$
- Matrix element: $A_{mn} = \int_{space} \psi_m^* \hat{A} \psi_n dx$
- Hermiticity condition:

$$A_{mn} = A_{nm}^* \rightarrow \int \psi_m^* \hat{A} \psi_n dx = \left(\int \psi_n^* \hat{A} \psi_m dx \right)^*$$

Dirac notation

"Ket" vector: $|\psi\rangle$

"Bra" vector: $\langle\psi| = |\psi\rangle^*$

"Bracket": $\langle\psi|\psi\rangle$

Complete sets: $\langle\psi_n|\psi_m\rangle = \delta_{nm}$

Eigenvalue equation: $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$

Superposition of states:

$$|\Psi\rangle = \sum_n c_n|\psi_n\rangle \rightarrow |\Psi\rangle^* = \langle\Psi| = \sum_n c_n^* \langle\psi_n$$

Overlap integral: $\langle\Psi|\Phi\rangle$ satisfies $\langle\Phi|\Psi\rangle^*$

Matrix element: $A_{mn} = \left\langle \psi_m \middle| \hat{A} \middle| \psi_n \right\rangle$

Hermiticity condition:

$$A_{mn} = A_{nm}^* \rightarrow \left\langle \psi_m \middle| \hat{A} \middle| \psi_n \right\rangle = \left\langle \psi_n \middle| \hat{A} \middle| \psi_m \right\rangle^*$$